WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 27, 2020 – 07:48 pm BST

PDB ID	:	2I3Z
Title	:	rat DPP-IV with xanthine mimetic inhibitor #7
Authors	:	Kurukulasuriya, R.; Rohde, J.J.; Szczepankiewicz, B.G.; Basha, F.; Lai, C.; Winn, M.; Stewart, K.D.; Longenecker, K.L.; Lubben, T.W.; Ballaron, S.J.; Sham, H.L.; VonGeldern, T.W.
Deposited on	:	2006-08-21
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (i)) were used in the production of this report:

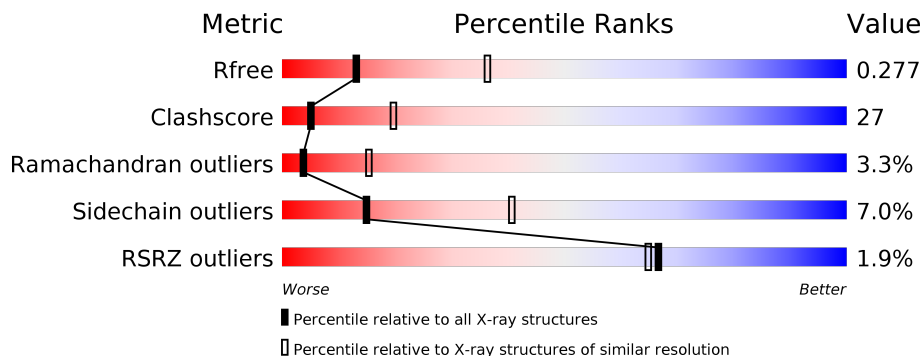|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.277
Clashscore		27
Ramachandran outliers		3.3%
Sidechain outliers		7.0%
RSRZ outliers		1.9%

Worse　　　　　　　　　　　　　　　　*Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

| Mol	Chain	Length	Quality of chain
1	A	730	54% · 39% · 6% ·
1	B	730	2% · 53% · 40% · 6% ·

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11867 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	730	Total 5920	C 3789	N 981	O 1124	S 26	0	0	0
1	B	730	Total 5920	C 3789	N 981	O 1124	S 26	0	0	0

- Molecule 2 is 2-[(3S)-3-AMINOPIPERIDIN-1-YL]-1-(2-CYANOBENZYL)-5-METHYL-4, 6-DIOXO-3,4,5,6-TETRAHYDROPYRROLO[3,4-D]IMIDAZOL-1-IUM (three-letter code: LIR) (formula: $C_{19}H_{21}N_6O_2$).
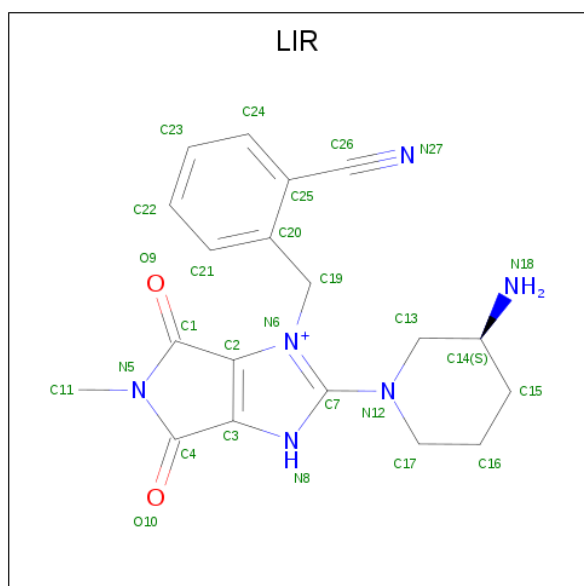

| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 27	C 19	N 6	O 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV)
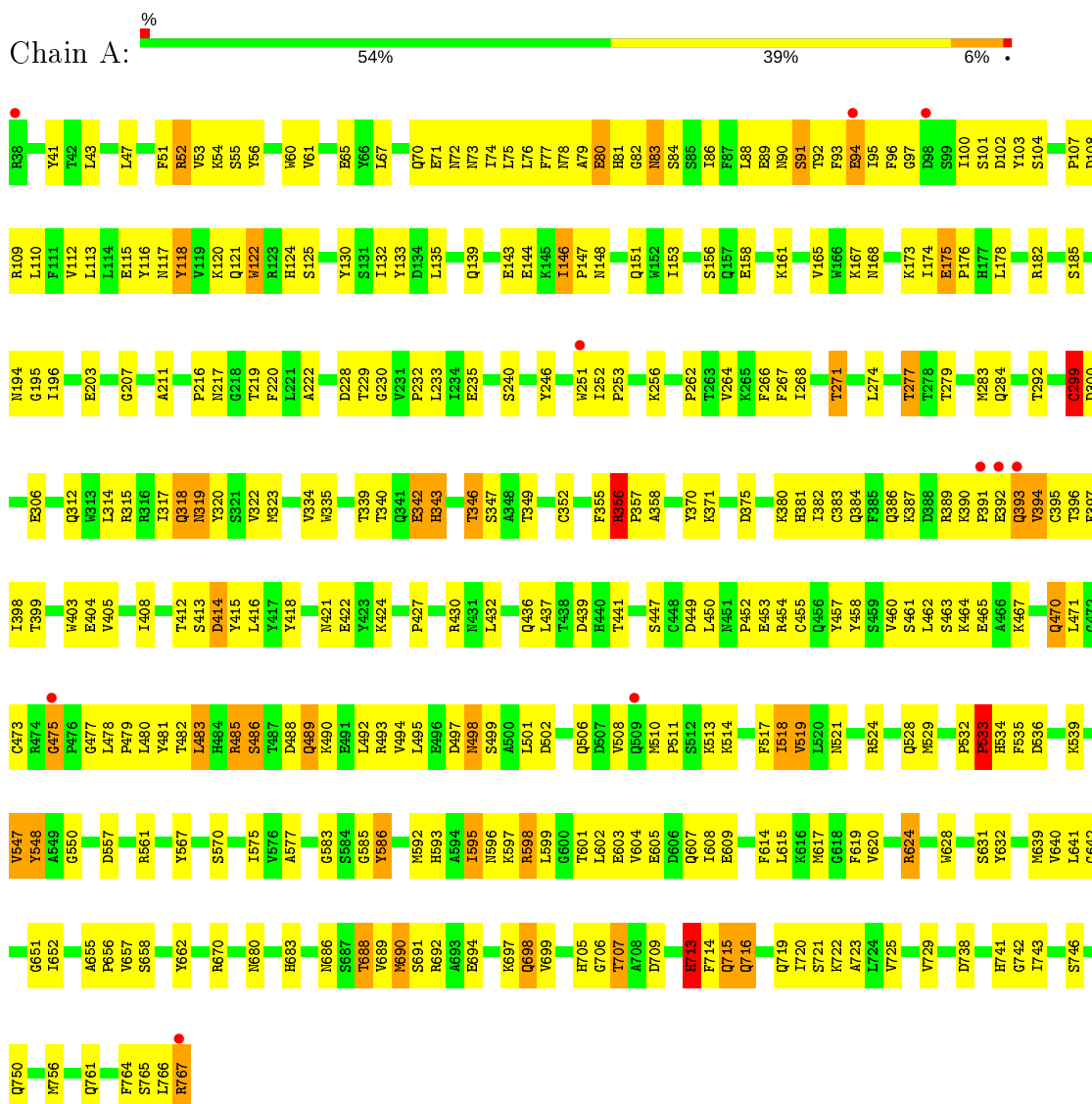
• Molecule 1: Dipeptidyl peptidase 4 (Dipeptidyl peptidase IV) (DPP IV)
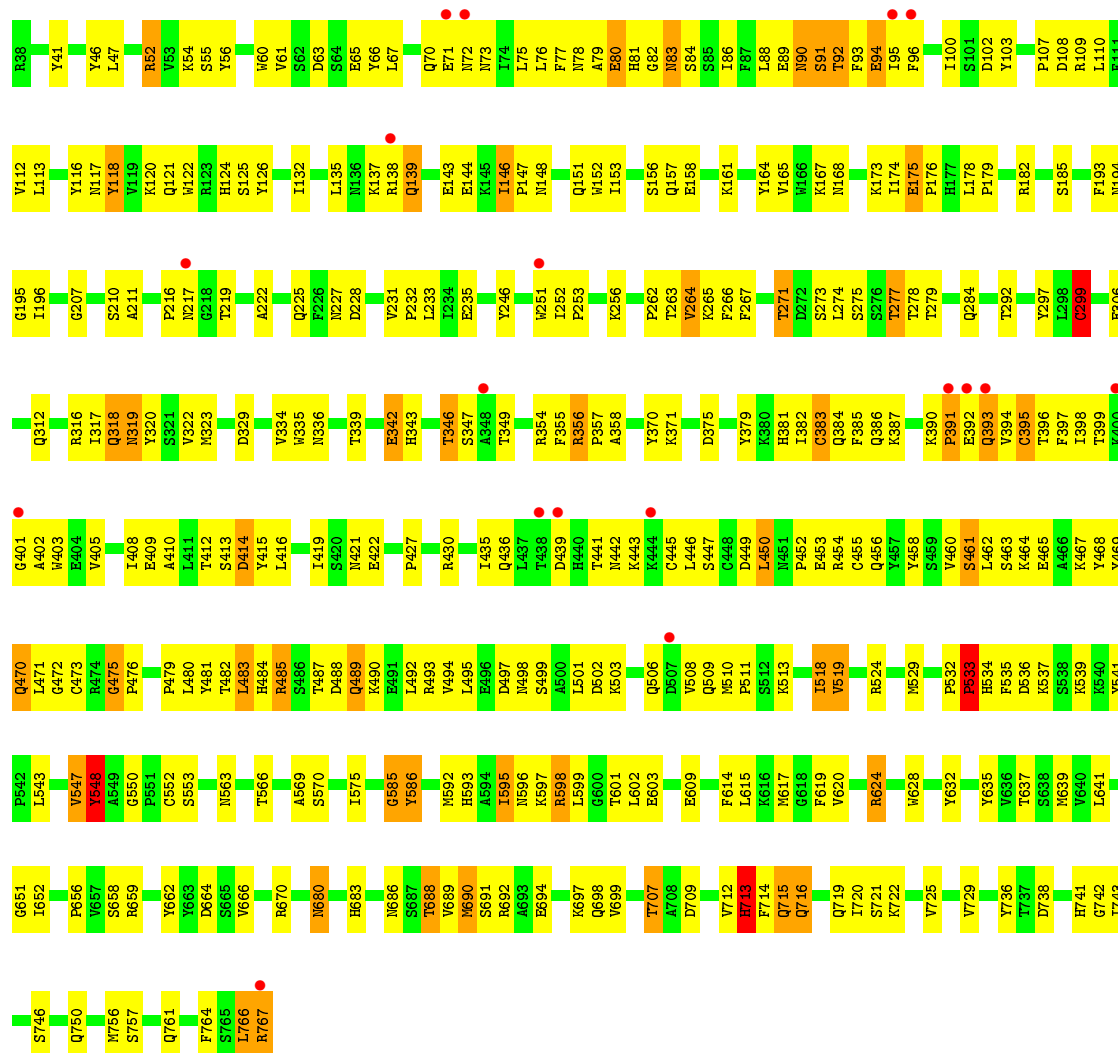
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α, β, γ	207.29Å 207.29Å 207.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 19.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-2.90) 99.7 (19.95-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.96 (at 2.88Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.253 , 0.290 0.240 , 0.277	Depositor DCC
R_{free} test set	3294 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.0	EDS
L-test for twinning[2]	$<|L|>$ = 0.52, $<L^2>$ = 0.36	Xtriage
Estimated twinning fraction	0.004 for l,-k,h	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	11867	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: LIR

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.51	2/6088 (0.0%)	0.73	2/8278 (0.0%)
1	B	0.54	1/6088 (0.0%)	0.73	5/8278 (0.1%)
All	All	0.52	3/12176 (0.0%)	0.73	7/16556 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	CYS	CB-SG	-6.05	1.72	1.82
1	A	352	CYS	CB-SG	-5.39	1.73	1.81
1	A	299	CYS	CB-SG	-5.27	1.73	1.81

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	713	HIS	N-CA-C	7.13	130.24	111.00
1	A	713	HIS	N-CA-C	6.90	129.63	111.00
1	B	548	TYR	N-CA-C	-6.11	94.50	111.00
1	A	548	TYR	N-CA-C	-6.07	94.61	111.00
1	B	585	GLY	N-CA-C	6.04	128.19	113.10
1	B	383	CYS	CA-CB-SG	5.18	123.32	114.00
1	B	90	ASN	N-CA-C	-5.07	97.30	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	736	TYR	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5920	0	5632	306	0
1	B	5920	0	5632	323	0
2	A	27	0	21	2	0
All	All	11867	0	11285	626	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 27.

All (626) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:ILE:HD11	1:A:603:GLU:HB3	1.33	1.10
1:A:52:ARG:HH11	1:A:52:ARG:HB2	1.21	1.05
1:B:595:ILE:HD11	1:B:603:GLU:HB3	1.37	1.02
1:A:349:THR:HB	1:A:593:HIS:HD2	1.22	1.02
1:B:235:GLU:HG2	1:B:251:TRP:HB3	1.41	1.01
1:A:91:SER:HA	1:A:94:GLU:OE1	1.61	1.01
1:B:349:THR:HB	1:B:593:HIS:HD2	1.27	0.99
1:A:412:THR:HG22	1:A:414:ASP:H	1.26	0.97
1:A:624:ARG:HB2	1:A:624:ARG:HH11	1.29	0.97
1:A:235:GLU:HG2	1:A:251:TRP:HB3	1.43	0.96
1:B:91:SER:HA	1:B:94:GLU:OE1	1.64	0.96
1:B:52:ARG:HB2	1:B:52:ARG:HH11	1.29	0.95
1:B:383:CYS:HB3	1:B:397:PHE:HA	1.49	0.95
1:A:383:CYS:HB3	1:A:397:PHE:HA	1.47	0.94
1:B:386:GLN:HG3	1:B:390:LYS:NZ	1.83	0.92
1:B:688:THR:HG22	1:B:691:SER:H	1.38	0.87
1:A:349:THR:HB	1:A:593:HIS:CD2	2.10	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:ASP:O	1:A:452:PRO:HD3	1.76	0.86
1:B:639:MET:HE3	1:B:689:VAL:HA	1.56	0.85
1:A:639:MET:HE3	1:A:689:VAL:HA	1.59	0.84
1:A:688:THR:HG22	1:A:691:SER:H	1.40	0.83
1:A:54:LYS:H	1:A:498:ASN:HD21	1.24	0.82
1:B:483:LEU:HB3	1:B:495:LEU:HD11	1.62	0.82
1:A:533:PRO:O	1:A:535:PHE:N	2.12	0.82
1:B:485:ARG:HB3	1:B:492:LEU:HD21	1.62	0.81
1:B:719:GLN:NE2	1:B:722:LYS:HE2	1.95	0.81
1:A:235:GLU:CG	1:A:251:TRP:HB3	2.09	0.81
1:A:52:ARG:HH11	1:A:52:ARG:CB	1.94	0.80
1:B:449:ASP:O	1:B:452:PRO:HD3	1.80	0.80
1:B:54:LYS:H	1:B:498:ASN:HD21	1.28	0.80
1:A:601:THR:HG22	1:A:602:LEU:N	1.97	0.79
1:B:697:LYS:HG2	1:B:729:VAL:HG22	1.64	0.79
1:A:386:GLN:HG3	1:A:390:LYS:NZ	1.97	0.79
1:B:235:GLU:CG	1:B:251:TRP:HB3	2.10	0.79
1:A:586:TYR:CD1	1:A:586:TYR:N	2.52	0.78
1:A:761:GLN:HB3	1:A:767:ARG:HB3	1.66	0.78
1:B:121:GLN:O	1:B:125:SER:HB2	1.85	0.77
1:A:690:MET:HE3	1:A:720:ILE:HA	1.67	0.77
1:A:79:ALA:O	1:A:80:GLU:HB2	1.86	0.76
1:B:79:ALA:O	1:B:80:GLU:HB2	1.86	0.76
1:B:78:ASN:HB3	1:B:83:ASN:HB3	1.68	0.76
1:A:639:MET:CE	1:A:689:VAL:HA	2.15	0.75
1:B:767:ARG:C	1:B:767:ARG:HD2	2.07	0.74
1:A:658:SER:H	1:A:716:GLN:HE21	1.33	0.74
1:A:80:GLU:H	1:A:493:ARG:HH22	1.34	0.74
1:A:624:ARG:HB2	1:A:624:ARG:NH1	2.02	0.74
1:B:408:ILE:HG23	1:B:416:LEU:HD11	1.68	0.74
1:B:460:VAL:HG22	1:B:461:SER:H	1.51	0.74
1:B:349:THR:HB	1:B:593:HIS:CD2	2.18	0.73
1:B:65:GLU:HB3	1:B:76:LEU:HD11	1.69	0.73
1:B:277:THR:HG21	1:B:279:THR:O	1.88	0.73
1:A:235:GLU:HG2	1:A:251:TRP:CB	2.19	0.73
1:B:761:GLN:HB3	1:B:767:ARG:HB3	1.70	0.73
1:B:54:LYS:H	1:B:498:ASN:ND2	1.88	0.72
1:B:174:ILE:HD12	1:B:174:ILE:H	1.52	0.72
1:A:277:THR:HG21	1:A:279:THR:O	1.90	0.72
1:A:381:HIS:CD2	1:A:399:THR:HG22	2.25	0.72
1:B:370:TYR:CE2	1:B:384:GLN:HG3	2.26	0.71

Full wwPDB X-ray Structure Validation Report

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:690:MET:CE	1:A:720:ILE:HA	2.21	0.71
1:A:121:GLN:O	1:A:125:SER:HB2	1.89	0.71
1:A:151:GLN:NE2	1:A:167:LYS:N	2.39	0.71
1:B:767:ARG:OXT	1:B:767:ARG:HD2	1.91	0.70
1:B:346:THR:HG23	1:B:347:SER:N	2.06	0.70
1:A:130:TYR:HB2	1:A:146:ILE:HD13	1.74	0.69
1:A:483:LEU:HB3	1:A:495:LEU:HD11	1.73	0.69
1:A:174:ILE:H	1:A:174:ILE:HD12	1.57	0.69
1:B:485:ARG:HG3	1:B:485:ARG:O	1.92	0.69
1:A:146:ILE:HD12	1:A:153:ILE:HD12	1.73	0.69
1:B:412:THR:HG22	1:B:414:ASP:H	1.58	0.69
1:B:55:SER:HA	1:B:481:TYR:CE1	2.28	0.69
1:A:658:SER:H	1:A:716:GLN:NE2	1.90	0.69
1:A:54:LYS:H	1:A:498:ASN:ND2	1.91	0.68
1:A:52:ARG:HB2	1:A:52:ARG:NH1	2.03	0.68
1:B:256:LYS:NZ	1:B:713:HIS:HD2	1.92	0.68
1:A:151:GLN:NE2	1:A:167:LYS:H	1.91	0.68
1:A:447:SER:HB2	1:A:458:TYR:CE1	2.29	0.68
1:A:101:SER:HB3	1:A:115:GLU:HG2	1.76	0.68
1:B:639:MET:CE	1:B:689:VAL:HA	2.24	0.68
1:A:460:VAL:HG22	1:A:461:SER:H	1.58	0.68
1:B:235:GLU:HG2	1:B:251:TRP:CB	2.20	0.68
1:A:370:TYR:CE2	1:A:384:GLN:HG3	2.28	0.67
1:B:158:GLU:HG2	1:B:217:ASN:HA	1.76	0.67
1:B:403:TRP:CE3	1:B:422:GLU:HB2	2.29	0.67
1:A:485:ARG:HB3	1:A:492:LEU:HD21	1.77	0.67
1:A:598:ARG:HE	1:A:601:THR:HG21	1.59	0.67
1:B:151:GLN:NE2	1:B:167:LYS:H	1.93	0.67
1:B:386:GLN:HG3	1:B:390:LYS:HZ2	1.57	0.67
1:A:78:ASN:HB3	1:A:83:ASN:HB3	1.75	0.67
1:A:694:GLU:O	1:A:697:LYS:HG3	1.95	0.66
1:A:55:SER:HA	1:A:481:TYR:CE1	2.30	0.66
1:B:502:ASP:O	1:B:506:GLN:HG2	1.96	0.66
1:A:412:THR:CG2	1:A:413:SER:N	2.58	0.66
1:A:392:GLU:C	1:A:393:GLN:HG3	2.17	0.66
1:B:447:SER:HB2	1:B:458:TYR:CE1	2.31	0.66
1:B:658:SER:H	1:B:716:GLN:NE2	1.93	0.66
1:B:52:ARG:CB	1:B:52:ARG:HH11	2.06	0.66
1:A:460:VAL:HG22	1:A:461:SER:N	2.10	0.65
1:B:586:TYR:N	1:B:586:TYR:CD1	2.62	0.65
1:A:151:GLN:HE22	1:A:168:ASN:H	1.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:ILE:HD12	1:B:153:ILE:HD12	1.79	0.65
1:B:61:VAL:CG2	1:B:67:LEU:HG	2.27	0.65
1:B:719:GLN:HE22	1:B:722:LYS:HE2	1.60	0.65
1:B:75:LEU:HB2	1:B:77:PHE:HE1	1.60	0.65
1:B:317:ILE:HG22	1:B:319:ASN:HB2	1.78	0.64
1:A:318:GLN:OE1	1:A:670:ARG:HD3	1.97	0.64
1:A:719:GLN:NE2	1:A:722:LYS:HE2	2.12	0.64
1:B:460:VAL:HG22	1:B:461:SER:N	2.12	0.64
1:A:597:LYS:O	1:A:683:HIS:HD2	1.81	0.64
1:B:386:GLN:HG3	1:B:390:LYS:HZ1	1.63	0.64
1:B:767:ARG:HH11	1:B:767:ARG:HG3	1.62	0.64
1:A:485:ARG:HG3	1:A:485:ARG:O	1.96	0.64
1:A:713:HIS:O	1:A:715:GLN:N	2.30	0.64
1:B:80:GLU:H	1:B:493:ARG:HH22	1.46	0.64
1:A:532:PRO:O	1:A:533:PRO:O	2.15	0.64
1:A:624:ARG:HH11	1:A:624:ARG:CB	2.08	0.64
1:B:392:GLU:C	1:B:393:GLN:HG3	2.18	0.64
1:B:690:MET:HE3	1:B:720:ILE:HA	1.80	0.64
1:B:690:MET:CE	1:B:720:ILE:HA	2.28	0.64
1:B:151:GLN:NE2	1:B:167:LYS:N	2.46	0.64
1:B:694:GLU:O	1:B:697:LYS:HG3	1.97	0.64
1:A:601:THR:HG22	1:A:602:LEU:H	1.62	0.63
1:B:75:LEU:HD23	1:B:86:ILE:HA	1.79	0.63
1:B:766:LEU:O	1:B:767:ARG:O	2.16	0.63
1:A:403:TRP:CE3	1:A:422:GLU:HB2	2.34	0.63
1:A:151:GLN:HE21	1:A:167:LYS:H	1.47	0.63
1:A:355:PHE:O	1:A:356:ARG:HB3	1.98	0.63
1:A:721:SER:O	1:A:725:VAL:HG23	1.99	0.62
1:B:639:MET:HE2	1:B:639:MET:HA	1.81	0.62
1:A:91:SER:O	1:A:93:PHE:N	2.33	0.62
1:B:598:ARG:HE	1:B:601:THR:HG21	1.65	0.62
1:A:381:HIS:CD2	1:A:399:THR:CG2	2.82	0.62
1:A:502:ASP:O	1:A:506:GLN:HG2	2.00	0.62
1:A:485:ARG:NH2	1:A:490:LYS:HD3	2.15	0.61
1:A:165:VAL:HG21	1:A:196:ILE:HG23	1.82	0.61
1:A:235:GLU:OE2	1:A:251:TRP:HB3	2.01	0.61
1:A:408:ILE:HG23	1:A:416:LEU:HD11	1.81	0.61
1:A:698:GLN:O	1:A:699:VAL:HG23	2.00	0.61
1:A:392:GLU:O	1:A:393:GLN:HG3	2.01	0.61
1:A:767:ARG:HG3	1:A:767:ARG:HH11	1.66	0.61
1:B:235:GLU:OE2	1:B:251:TRP:HB3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:547:VAL:HG23	1:B:628:TRP:O	2.00	0.61
1:A:518:ILE:HD13	1:A:519:VAL:H	1.64	0.61
1:B:597:LYS:O	1:B:683:HIS:HD2	1.84	0.60
1:A:158:GLU:HG2	1:A:217:ASN:HA	1.83	0.60
1:B:108:ASP:OD2	1:B:110:LEU:HD12	2.01	0.60
1:B:488:ASP:O	1:B:489:GLN:HB2	2.00	0.60
1:A:536:ASP:OD2	1:A:539:LYS:HG3	2.01	0.60
1:A:412:THR:HG22	1:A:414:ASP:N	2.08	0.60
1:A:54:LYS:N	1:A:498:ASN:HD21	1.97	0.60
1:A:61:VAL:HG21	1:A:67:LEU:HG	1.83	0.60
1:A:641:LEU:HD11	1:A:651:GLY:HA3	1.81	0.60
1:B:151:GLN:HE22	1:B:168:ASN:H	1.49	0.60
1:B:70:GLN:HG2	1:B:71:GLU:HG3	1.82	0.60
1:A:219:THR:O	1:A:271:THR:HB	2.02	0.60
1:B:256:LYS:HZ1	1:B:713:HIS:HD2	1.50	0.60
1:A:79:ALA:O	1:A:80:GLU:CB	2.50	0.59
1:B:358:ALA:O	1:B:371:LYS:HE3	2.01	0.59
1:A:75:LEU:HB2	1:A:77:PHE:HE1	1.67	0.59
1:A:323:MET:O	1:A:342:GLU:O	2.21	0.59
1:B:267:PHE:CE2	1:B:284:GLN:HB2	2.38	0.59
1:B:601:THR:HG22	1:B:602:LEU:N	2.16	0.59
1:B:624:ARG:HB2	1:B:624:ARG:HH11	1.67	0.59
1:B:767:ARG:CD	1:B:767:ARG:OXT	2.50	0.59
1:A:267:PHE:CE2	1:A:284:GLN:HB2	2.37	0.59
1:A:412:THR:HG22	1:A:413:SER:N	2.18	0.59
1:B:485:ARG:NH2	1:B:490:LYS:HD3	2.17	0.59
1:B:498:ASN:HB3	1:B:501:LEU:HB3	1.85	0.59
1:A:88:LEU:HD11	1:A:112:VAL:HG11	1.83	0.59
1:A:233:LEU:HD23	1:A:253:PRO:HA	1.85	0.59
1:B:151:GLN:HE21	1:B:167:LYS:H	1.48	0.58
1:B:658:SER:H	1:B:716:GLN:HE21	1.51	0.58
1:B:61:VAL:HG21	1:B:67:LEU:HG	1.84	0.58
1:B:688:THR:HG23	1:B:690:MET:HG2	1.84	0.58
1:B:713:HIS:C	1:B:715:GLN:H	2.06	0.58
1:B:91:SER:O	1:B:93:PHE:N	2.36	0.58
1:A:256:LYS:NZ	1:A:713:HIS:HD2	2.01	0.58
1:B:518:ILE:HD13	1:B:519:VAL:H	1.68	0.58
1:B:767:ARG:HG3	1:B:767:ARG:NH1	2.18	0.58
1:B:54:LYS:N	1:B:498:ASN:HD21	2.00	0.58
1:A:536:ASP:HB3	1:A:539:LYS:HE2	1.86	0.58
1:A:688:THR:CG2	1:A:690:MET:HG2	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:THR:O	1:B:342:GLU:HB2	2.04	0.57
1:A:497:ASP:O	1:A:499:SER:N	2.36	0.57
1:A:690:MET:HE1	1:A:720:ILE:N	2.19	0.57
1:A:709:ASP:OD2	1:A:741:HIS:HA	2.04	0.57
1:B:381:HIS:CD2	1:B:399:THR:HG22	2.40	0.57
1:B:533:PRO:O	1:B:535:PHE:N	2.29	0.57
1:A:662:TYR:OH	1:A:719:GLN:HG2	2.05	0.57
1:A:713:HIS:C	1:A:715:GLN:H	2.07	0.57
1:B:713:HIS:O	1:B:714:PHE:HB3	2.05	0.57
1:A:235:GLU:CD	1:A:251:TRP:HB3	2.24	0.57
1:B:107:PRO:HG2	1:B:158:GLU:O	2.04	0.57
1:B:401:GLY:HA3	1:B:403:TRP:NE1	2.20	0.57
1:A:598:ARG:HD3	1:A:598:ARG:O	2.03	0.56
1:A:639:MET:HE2	1:A:639:MET:HA	1.87	0.56
1:A:339:THR:O	1:A:342:GLU:HB2	2.05	0.56
1:A:41:TYR:HB2	1:A:510:MET:HE2	1.87	0.56
1:B:532:PRO:O	1:B:533:PRO:O	2.23	0.56
1:B:662:TYR:OH	1:B:719:GLN:HG2	2.05	0.56
1:B:346:THR:CG2	1:B:347:SER:N	2.68	0.56
1:A:624:ARG:NH1	1:A:624:ARG:CB	2.68	0.56
1:A:688:THR:HG23	1:A:690:MET:HG2	1.87	0.56
1:A:375:ASP:HA	1:A:397:PHE:CZ	2.41	0.56
1:B:370:TYR:HE2	1:B:398:ILE:CD1	2.19	0.56
1:A:216:PRO:O	1:A:217:ASN:HB2	2.05	0.56
1:A:421:ASN:ND2	1:A:427:PRO:HA	2.20	0.56
1:B:381:HIS:CD2	1:B:399:THR:CG2	2.89	0.56
1:B:375:ASP:HA	1:B:397:PHE:CZ	2.41	0.56
1:B:323:MET:O	1:B:342:GLU:O	2.24	0.56
1:B:355:PHE:O	1:B:356:ARG:HB3	2.06	0.56
1:B:688:THR:HG22	1:B:691:SER:N	2.15	0.56
1:A:61:VAL:CG2	1:A:67:LEU:HG	2.35	0.55
1:A:536:ASP:HB3	1:A:539:LYS:NZ	2.21	0.55
1:B:680:ASN:HD21	1:B:683:HIS:CD2	2.24	0.55
1:B:688:THR:CG2	1:B:690:MET:HG2	2.37	0.55
1:B:482:THR:HG22	1:B:494:VAL:HG22	1.87	0.55
1:A:398:ILE:O	1:A:398:ILE:HG22	2.07	0.55
1:A:498:ASN:HB3	1:A:501:LEU:HB3	1.88	0.55
1:B:615:LEU:HD23	1:B:620:VAL:CG1	2.37	0.55
1:A:586:TYR:HD1	1:A:586:TYR:H	1.54	0.55
1:A:639:MET:HE3	1:A:689:VAL:CA	2.34	0.54
1:A:89:GLU:C	1:A:91:SER:N	2.57	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:HIS:O	1:A:83:ASN:N	2.41	0.54
1:A:601:THR:HG22	1:A:602:LEU:HD23	1.89	0.54
1:A:536:ASP:CB	1:A:539:LYS:NZ	2.70	0.54
1:B:277:THR:HG22	1:B:278:THR:H	1.71	0.54
1:B:72:ASN:O	1:B:90:ASN:HA	2.07	0.54
1:A:547:VAL:HG23	1:A:628:TRP:O	2.07	0.54
1:A:317:ILE:HG22	1:A:319:ASN:HB2	1.90	0.54
1:A:41:TYR:HB2	1:A:510:MET:CE	2.38	0.54
1:B:513:LYS:HA	1:B:529:MET:O	2.07	0.54
1:B:652:ILE:HG21	1:B:756:MET:HE2	1.90	0.53
1:B:742:GLY:O	1:B:743:ILE:C	2.46	0.53
1:B:320:TYR:CE2	1:B:322:VAL:HG23	2.43	0.53
1:B:79:ALA:O	1:B:80:GLU:CB	2.56	0.53
1:A:320:TYR:CE2	1:A:322:VAL:HG23	2.43	0.53
1:B:219:THR:O	1:B:271:THR:HB	2.08	0.53
1:A:383:CYS:HB3	1:A:397:PHE:CA	2.30	0.53
1:B:698:GLN:O	1:B:699:VAL:HG23	2.08	0.53
1:A:151:GLN:HE22	1:A:167:LYS:N	2.07	0.53
1:A:346:THR:HG23	1:A:347:SER:N	2.23	0.53
1:B:473:CYS:O	1:B:479:PRO:HA	2.09	0.53
1:B:60:TRP:CE3	1:B:66:TYR:HB3	2.44	0.53
1:B:719:GLN:HE22	1:B:722:LYS:CE	2.20	0.53
1:A:415:TYR:HD2	1:A:436:GLN:HA	1.73	0.53
1:A:513:LYS:HA	1:A:529:MET:O	2.08	0.52
1:A:628:TRP:CE3	1:A:756:MET:HE1	2.44	0.52
1:A:70:GLN:HG2	1:A:71:GLU:HG3	1.92	0.52
1:A:256:LYS:HZ3	1:A:713:HIS:HD2	1.56	0.52
1:B:757:SER:O	1:B:761:GLN:HG3	2.10	0.52
1:B:88:LEU:HD11	1:B:112:VAL:HG11	1.91	0.52
1:A:382:ILE:HG13	1:A:405:VAL:HG21	1.91	0.52
1:B:235:GLU:CD	1:B:251:TRP:HB3	2.29	0.52
1:B:415:TYR:HD2	1:B:436:GLN:HA	1.75	0.52
1:B:506:GLN:HA	1:B:506:GLN:OE1	2.10	0.52
1:B:639:MET:HE3	1:B:689:VAL:CA	2.34	0.52
1:A:455:CYS:HA	1:A:475:GLY:HA3	1.91	0.52
1:A:761:GLN:HB3	1:A:767:ARG:CB	2.39	0.52
1:A:403:TRP:CD2	1:A:422:GLU:HB2	2.45	0.52
1:A:614:PHE:O	1:A:617:MET:HB2	2.10	0.52
1:B:318:GLN:NE2	1:B:670:ARG:HB2	2.25	0.51
1:B:63:ASP:CG	1:B:465:GLU:HB2	2.31	0.51
1:A:168:ASN:O	1:A:194:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PHE:CD2	1:A:100:ILE:HG21	2.46	0.51
1:A:767:ARG:NH1	1:A:767:ARG:HG3	2.26	0.51
1:A:108:ASP:OD2	1:A:110:LEU:HD12	2.11	0.51
1:B:412:THR:HG22	1:B:413:SER:N	2.25	0.51
1:A:277:THR:CG2	1:A:279:THR:O	2.58	0.51
1:B:222:ALA:HB1	1:B:266:PHE:CZ	2.46	0.51
1:B:598:ARG:HD3	1:B:598:ARG:O	2.11	0.51
1:B:75:LEU:HB2	1:B:77:PHE:CE1	2.44	0.51
1:A:536:ASP:HB3	1:A:539:LYS:CE	2.40	0.51
1:B:60:TRP:CG	1:B:463:SER:HA	2.46	0.51
1:B:482:THR:OG1	1:B:484:HIS:HE1	1.93	0.51
1:B:403:TRP:CD2	1:B:422:GLU:HB2	2.45	0.50
1:B:370:TYR:CE2	1:B:398:ILE:CD1	2.94	0.50
1:A:132:ILE:HG21	1:A:176:PRO:HB3	1.93	0.50
1:A:688:THR:HG22	1:A:691:SER:N	2.18	0.50
1:B:227:ASN:HB3	1:B:263:THR:OG1	2.11	0.50
1:B:299:CYS:SG	1:B:357:PRO:HD2	2.52	0.50
1:B:485:ARG:O	1:B:485:ARG:CG	2.60	0.50
1:A:454:ARG:HD3	1:A:478:LEU:O	2.11	0.50
1:B:447:SER:HB2	1:B:458:TYR:CD1	2.46	0.50
1:A:299:CYS:HB2	1:A:312:GLN:O	2.12	0.50
1:A:383:CYS:HB2	1:A:396:THR:C	2.32	0.50
1:B:161:LYS:NZ	1:B:271:THR:CG2	2.75	0.50
1:B:624:ARG:NH1	1:B:624:ARG:HB2	2.27	0.50
1:B:113:LEU:HD23	1:B:132:ILE:HD13	1.94	0.50
1:B:412:THR:CG2	1:B:413:SER:N	2.75	0.50
1:A:342:GLU:O	1:A:343:HIS:HB2	2.12	0.50
1:A:383:CYS:CB	1:A:397:PHE:HA	2.31	0.50
1:B:548:TYR:CD2	1:B:553:SER:HB2	2.47	0.50
1:B:680:ASN:HD21	1:B:683:HIS:CG	2.30	0.50
1:A:228:ASP:OD1	1:A:262:PRO:HB3	2.12	0.50
1:A:467:LYS:O	1:A:486:SER:HB2	2.11	0.50
1:A:235:GLU:OE2	1:A:251:TRP:CD1	2.65	0.49
1:A:47:LEU:HD22	1:A:750:GLN:HA	1.93	0.49
1:B:383:CYS:HB3	1:B:397:PHE:CA	2.32	0.49
1:A:156:SER:HB3	1:A:161:LYS:HB2	1.94	0.49
1:A:75:LEU:HD23	1:A:86:ILE:HA	1.94	0.49
1:A:229:THR:HG22	1:A:230:GLY:N	2.27	0.49
1:B:132:ILE:HG21	1:B:176:PRO:HB3	1.94	0.49
1:B:56:TYR:CE2	1:B:495:LEU:HD22	2.46	0.49
1:B:116:TYR:O	1:B:117:ASN:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:GLU:HG3	1:B:460:VAL:HG11	1.94	0.49
1:B:467:LYS:HD3	1:B:468:TYR:HE1	1.77	0.49
1:B:529:MET:CE	1:B:575:ILE:HG21	2.43	0.49
1:A:80:GLU:N	1:A:493:ARG:HH22	2.07	0.49
1:A:690:MET:CE	1:A:720:ILE:CA	2.91	0.49
1:A:697:LYS:HG2	1:A:729:VAL:HG22	1.94	0.49
1:A:158:GLU:OE2	1:A:217:ASN:N	2.45	0.49
1:B:470:GLN:HG2	1:B:471:LEU:N	2.28	0.49
1:B:228:ASP:OD1	1:B:262:PRO:HB3	2.11	0.49
1:B:595:ILE:HG23	1:B:599:LEU:HD23	1.95	0.49
1:A:203:GLU:OE2	2:A:900:LIR:N18	2.46	0.49
1:A:386:GLN:HG3	1:A:390:LYS:HZ1	1.73	0.49
1:A:488:ASP:O	1:A:489:GLN:HB2	2.13	0.49
1:A:80:GLU:HA	1:A:492:LEU:HD13	1.95	0.49
1:A:657:VAL:HG13	1:A:716:GLN:HE22	1.78	0.49
1:B:548:TYR:C	1:B:548:TYR:CD1	2.86	0.49
1:B:118:TYR:C	1:B:118:TYR:CD2	2.85	0.49
1:B:137:LYS:O	1:B:139:GLN:HG3	2.13	0.49
1:A:386:GLN:HG3	1:A:390:LYS:CE	2.43	0.48
1:A:601:THR:CG2	1:A:602:LEU:H	2.23	0.48
1:B:419:ILE:HD11	1:B:460:VAL:HG12	1.95	0.48
1:A:107:PRO:HG2	1:A:158:GLU:O	2.14	0.48
1:A:195:GLY:C	1:A:211:ALA:HB3	2.34	0.48
1:A:216:PRO:O	1:A:306:GLU:HG3	2.14	0.48
1:B:168:ASN:O	1:B:194:ASN:HB2	2.14	0.48
1:B:441:THR:O	1:B:443:LYS:N	2.43	0.48
1:B:709:ASP:OD2	1:B:741:HIS:HA	2.13	0.48
1:A:482:THR:HG22	1:A:494:VAL:HG22	1.94	0.48
1:B:96:PHE:CB	1:B:100:ILE:HD11	2.43	0.48
1:B:536:ASP:HB3	1:B:539:LYS:NZ	2.28	0.48
1:B:89:GLU:C	1:B:91:SER:N	2.66	0.48
1:A:65:GLU:HB3	1:A:76:LEU:HD11	1.95	0.48
1:B:216:PRO:O	1:B:217:ASN:HB2	2.14	0.48
1:B:467:LYS:HD3	1:B:468:TYR:CE1	2.48	0.48
1:A:597:LYS:O	1:A:683:HIS:CD2	2.65	0.48
1:A:122:TRP:CE3	1:A:122:TRP:N	2.81	0.48
1:A:765:SER:HA	1:A:767:ARG:HH12	1.78	0.48
1:B:456:GLN:OE1	1:B:476:PRO:HG2	2.13	0.48
1:B:532:PRO:HB3	1:B:569:ALA:O	2.13	0.48
1:B:652:ILE:HG21	1:B:756:MET:CE	2.43	0.48
1:A:116:TYR:O	1:A:117:ASN:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:TYR:HB2	1:B:510:MET:HE2	1.95	0.48
1:A:624:ARG:HG2	1:A:764:PHE:CD2	2.49	0.48
1:B:455:CYS:HA	1:B:475:GLY:HA3	1.94	0.48
1:A:641:LEU:HD22	1:A:699:VAL:HG11	1.95	0.47
1:A:742:GLY:O	1:A:743:ILE:C	2.52	0.47
1:B:392:GLU:O	1:B:393:GLN:HG3	2.14	0.47
1:B:652:ILE:CD1	1:B:756:MET:HE2	2.44	0.47
1:A:124:HIS:CE1	1:A:207:GLY:O	2.68	0.47
1:B:408:ILE:CG2	1:B:416:LEU:HD11	2.40	0.47
1:A:315:ARG:HD2	1:A:320:TYR:HB3	1.96	0.47
1:A:547:VAL:HG13	1:A:607:GLN:OE1	2.15	0.47
1:B:235:GLU:OE2	1:B:251:TRP:CD1	2.67	0.47
1:B:312:GLN:HG2	1:B:323:MET:HG3	1.97	0.47
1:A:222:ALA:HB1	1:A:266:PHE:CZ	2.50	0.47
1:A:454:ARG:HG2	1:A:477:GLY:HA3	1.96	0.47
1:A:533:PRO:HD3	1:A:570:SER:HA	1.95	0.47
1:B:233:LEU:HD23	1:B:253:PRO:HA	1.97	0.47
1:B:41:TYR:CD2	1:B:566:THR:HG22	2.50	0.47
1:B:462:LEU:N	1:B:462:LEU:HD12	2.30	0.47
1:B:70:GLN:O	1:B:73:ASN:HB2	2.15	0.47
1:A:317:ILE:C	1:A:319:ASN:H	2.17	0.47
1:A:412:THR:CG2	1:A:413:SER:H	2.27	0.47
1:A:447:SER:HB2	1:A:458:TYR:CD1	2.49	0.47
1:B:597:LYS:O	1:B:683:HIS:CD2	2.66	0.47
1:B:78:ASN:O	1:B:81:HIS:O	2.33	0.47
1:A:104:SER:HB3	1:A:113:LEU:HB2	1.97	0.47
1:A:120:LYS:CG	1:A:121:GLN:N	2.77	0.47
1:A:657:VAL:HA	1:A:716:GLN:NE2	2.29	0.47
1:B:382:ILE:HG13	1:B:405:VAL:HG21	1.97	0.47
1:A:439:ASP:OD1	1:A:441:THR:HB	2.14	0.47
1:A:462:LEU:N	1:A:462:LEU:HD12	2.29	0.47
1:A:707:THR:CG2	1:A:738:ASP:H	2.27	0.47
1:B:485:ARG:HG2	1:B:488:ASP:OD1	2.15	0.47
1:B:632:TYR:O	1:B:635:TYR:HB3	2.15	0.47
1:A:536:ASP:CB	1:A:539:LYS:HZ1	2.28	0.47
1:A:631:SER:HB2	2:A:900:LIR:O9	2.15	0.47
1:B:158:GLU:HG2	1:B:217:ASN:CA	2.44	0.47
1:A:349:THR:CB	1:A:593:HIS:HD2	2.09	0.47
1:B:267:PHE:CD2	1:B:284:GLN:HB2	2.50	0.47
1:B:292:THR:O	1:B:292:THR:HG22	2.13	0.47
1:B:436:GLN:OE1	1:B:439:ASP:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:ARG:HH11	1:B:524:ARG:HG2	1.80	0.47
1:B:548:TYR:CE1	1:B:550:GLY:HA3	2.50	0.47
1:B:624:ARG:HG2	1:B:764:PHE:CD2	2.49	0.47
1:B:641:LEU:HD11	1:B:651:GLY:HA3	1.95	0.47
1:A:370:TYR:CE2	1:A:384:GLN:CG	2.97	0.46
1:A:550:GLY:HA2	1:A:632:TYR:CE2	2.50	0.46
1:A:72:ASN:O	1:A:90:ASN:HA	2.15	0.46
1:B:454:ARG:NH1	1:B:480:LEU:HB2	2.30	0.46
1:A:151:GLN:HE22	1:A:168:ASN:N	2.12	0.46
1:A:583:GLY:HA3	1:A:595:ILE:HD12	1.98	0.46
1:A:761:GLN:CB	1:A:767:ARG:HB3	2.42	0.46
1:B:109:ARG:O	1:B:135:LEU:HD12	2.15	0.46
1:B:152:TRP:CE2	1:B:210:SER:HB2	2.50	0.46
1:B:595:ILE:HD11	1:B:603:GLU:CB	2.27	0.46
1:A:151:GLN:NE2	1:A:168:ASN:H	2.13	0.46
1:B:386:GLN:HG3	1:B:390:LYS:CE	2.43	0.46
1:A:118:TYR:C	1:A:118:TYR:CD2	2.88	0.46
1:A:460:VAL:CG2	1:A:461:SER:H	2.26	0.46
1:A:596:ASN:O	1:A:598:ARG:HG3	2.15	0.46
1:A:470:GLN:HG2	1:A:471:LEU:N	2.30	0.46
1:A:713:HIS:O	1:A:714:PHE:HB3	2.16	0.46
1:A:746:SER:O	1:A:750:GLN:HG3	2.16	0.46
1:A:174:ILE:HD12	1:A:174:ILE:N	2.28	0.46
1:A:497:ASP:O	1:A:497:ASP:CG	2.54	0.46
1:A:529:MET:CE	1:A:575:ILE:HG21	2.46	0.46
1:A:267:PHE:CD2	1:A:284:GLN:HB2	2.50	0.46
1:A:615:LEU:HD23	1:A:620:VAL:CG1	2.45	0.46
1:B:161:LYS:HZ3	1:B:271:THR:CG2	2.29	0.46
1:B:175:GLU:HG3	1:B:178:LEU:HG	1.98	0.46
1:B:536:ASP:HB3	1:B:539:LYS:HE2	1.97	0.46
1:B:552:CYS:HB2	1:B:592:MET:SD	2.55	0.46
1:A:41:TYR:HE1	1:A:51:PHE:HD1	1.62	0.46
1:B:41:TYR:HB2	1:B:510:MET:CE	2.44	0.46
1:B:541:TYR:CD1	1:B:541:TYR:N	2.84	0.46
1:B:690:MET:HE2	1:B:719:GLN:O	2.15	0.46
1:A:299:CYS:SG	1:A:357:PRO:HD2	2.56	0.46
1:A:415:TYR:CD2	1:A:436:GLN:HA	2.51	0.46
1:A:595:ILE:HG23	1:A:599:LEU:HD23	1.98	0.46
1:A:603:GLU:N	1:A:603:GLU:OE1	2.49	0.46
1:B:543:LEU:HD12	1:B:575:ILE:O	2.16	0.46
1:A:719:GLN:HE22	1:A:722:LYS:NZ	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ILE:C	1:B:319:ASN:H	2.19	0.45
1:B:713:HIS:C	1:B:715:GLN:N	2.70	0.45
1:B:385:PHE:CZ	1:B:395:CYS:SG	3.09	0.45
1:A:113:LEU:HD21	1:A:153:ILE:HD13	1.99	0.45
1:A:713:HIS:C	1:A:715:GLN:N	2.69	0.45
1:B:354:ARG:HD3	1:B:552:CYS:SG	2.57	0.45
1:B:297:TYR:CE2	1:B:666:VAL:HG22	2.51	0.45
1:A:292:THR:HG22	1:A:292:THR:O	2.16	0.45
1:B:144:GLU:HG3	1:B:179:PRO:N	2.31	0.45
1:B:688:THR:CG2	1:B:691:SER:H	2.20	0.45
1:A:473:CYS:O	1:A:479:PRO:HA	2.16	0.45
1:B:217:ASN:HB2	1:B:306:GLU:OE2	2.17	0.45
1:B:318:GLN:HE22	1:B:670:ARG:HB2	1.81	0.45
1:A:386:GLN:HG3	1:A:390:LYS:HZ2	1.77	0.45
1:B:157:GLN:HB2	1:B:158:GLU:OE2	2.17	0.45
1:A:467:LYS:C	1:A:486:SER:HB2	2.37	0.45
1:B:81:HIS:C	1:B:83:ASN:H	2.20	0.45
1:A:74:ILE:HB	1:A:88:LEU:HB2	1.98	0.45
1:B:156:SER:HB3	1:B:161:LYS:HB2	1.98	0.45
1:B:460:VAL:CG2	1:B:461:SER:H	2.25	0.45
1:B:652:ILE:HD13	1:B:756:MET:HE2	1.99	0.45
1:B:624:ARG:HG2	1:B:764:PHE:HD2	1.82	0.45
1:A:529:MET:HG2	1:A:577:ALA:HB2	1.98	0.45
1:B:401:GLY:HA3	1:B:403:TRP:HE1	1.81	0.45
1:B:445:CYS:C	1:B:446:LEU:HD23	2.38	0.45
1:B:482:THR:HG22	1:B:494:VAL:HA	1.98	0.45
1:A:583:GLY:HA2	1:A:592:MET:O	2.18	0.44
1:A:690:MET:HB3	1:A:723:ALA:HB2	1.98	0.44
1:A:96:PHE:CB	1:A:100:ILE:HD11	2.47	0.44
1:B:439:ASP:OD1	1:B:441:THR:HB	2.16	0.44
1:A:601:THR:HG22	1:A:602:LEU:CD2	2.47	0.44
1:A:60:TRP:CG	1:A:463:SER:HA	2.53	0.44
1:B:392:GLU:O	1:B:393:GLN:CG	2.65	0.44
1:B:391:PRO:O	1:B:393:GLN:HG3	2.17	0.44
1:B:398:ILE:HG22	1:B:398:ILE:O	2.17	0.44
1:B:410:ALA:O	1:B:416:LEU:HD12	2.17	0.44
1:B:659:ARG:HG2	1:B:662:TYR:CE2	2.53	0.44
1:A:334:VAL:CG1	1:A:335:TRP:N	2.80	0.44
1:A:460:VAL:CG2	1:A:461:SER:N	2.79	0.44
1:B:125:SER:O	1:B:126:TYR:HB3	2.16	0.44
1:A:506:GLN:HA	1:A:506:GLN:OE1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:ARG:HD2	1:B:487:THR:HB	1.99	0.44
1:B:46:TYR:CE1	1:B:563:ASN:HA	2.52	0.44
1:B:596:ASN:O	1:B:598:ARG:HG3	2.18	0.44
1:B:614:PHE:O	1:B:617:MET:HB2	2.17	0.44
1:A:511:PRO:HD3	1:A:570:SER:HB2	2.00	0.44
1:A:342:GLU:HB3	1:A:389:ARG:HH21	1.81	0.44
1:A:628:TRP:CE3	1:A:756:MET:CE	3.01	0.44
1:A:658:SER:HB2	1:A:690:MET:SD	2.57	0.44
1:A:705:HIS:CD2	1:A:706:GLY:N	2.86	0.44
1:B:306:GLU:O	1:B:306:GLU:HG2	2.17	0.44
1:A:412:THR:HG23	1:A:413:SER:H	1.82	0.44
1:A:52:ARG:HH11	1:A:52:ARG:CG	2.30	0.44
1:A:595:ILE:CG2	1:A:599:LEU:HD23	2.48	0.44
1:B:231:VAL:HA	1:B:232:PRO:HD3	1.90	0.44
1:B:435:ILE:HG22	1:B:436:GLN:N	2.32	0.44
1:A:122:TRP:CH2	1:A:252:ILE:HD11	2.53	0.43
1:A:421:ASN:HD22	1:A:427:PRO:HA	1.82	0.43
1:A:508:VAL:HG12	1:A:510:MET:HE3	1.99	0.43
1:B:470:GLN:HA	1:B:483:LEU:HA	1.99	0.43
1:B:91:SER:CA	1:B:94:GLU:OE1	2.50	0.43
1:A:766:LEU:O	1:A:767:ARG:NH1	2.46	0.43
1:B:719:GLN:HE22	1:B:722:LYS:NZ	2.16	0.43
1:A:232:PRO:HB2	1:B:246:TYR:CZ	2.53	0.43
1:A:312:GLN:HG2	1:A:323:MET:HG3	2.00	0.43
1:B:447:SER:HA	1:B:450:LEU:HD12	1.99	0.43
1:B:707:THR:CG2	1:B:738:ASP:H	2.31	0.43
1:B:318:GLN:OE1	1:B:670:ARG:HD3	2.19	0.43
1:B:690:MET:HE1	1:B:720:ILE:N	2.33	0.43
1:A:93:PHE:O	1:A:100:ILE:HG13	2.19	0.43
1:B:195:GLY:C	1:B:211:ALA:HB3	2.39	0.43
1:B:334:VAL:CG1	1:B:335:TRP:N	2.82	0.43
1:A:73:ASN:HD21	1:A:90:ASN:CG	2.22	0.43
1:B:165:VAL:HG21	1:B:196:ILE:HG23	1.99	0.43
1:B:386:GLN:O	1:B:387:LYS:C	2.55	0.43
1:A:102:ASP:OD1	1:A:103:TYR:N	2.45	0.43
1:A:81:HIS:C	1:A:83:ASN:H	2.22	0.43
1:B:383:CYS:CB	1:B:397:PHE:HA	2.33	0.43
1:B:103:TYR:HA	1:B:113:LEU:O	2.18	0.43
1:B:122:TRP:CH2	1:B:252:ILE:HD11	2.54	0.43
1:B:386:GLN:CG	1:B:390:LYS:HZ1	2.30	0.43
1:B:81:HIS:O	1:B:83:ASN:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:TYR:CE2	1:B:232:PRO:HB2	2.54	0.42
1:A:217:ASN:HB2	1:A:306:GLU:OE2	2.18	0.42
1:A:358:ALA:O	1:A:371:LYS:HE3	2.18	0.42
1:A:642:GLY:O	1:A:692:ARG:HB3	2.19	0.42
1:B:144:GLU:OE1	1:B:179:PRO:HB3	2.19	0.42
1:B:146:ILE:CD1	1:B:153:ILE:HD12	2.46	0.42
1:B:182:ARG:HH21	1:B:185:SER:HA	1.83	0.42
1:B:277:THR:HG22	1:B:278:THR:N	2.33	0.42
1:B:383:CYS:HB2	1:B:396:THR:O	2.19	0.42
1:B:719:GLN:NE2	1:B:722:LYS:CE	2.75	0.42
1:A:719:GLN:HE22	1:A:722:LYS:CE	2.32	0.42
1:B:586:TYR:HD1	1:B:586:TYR:H	1.65	0.42
1:B:761:GLN:CB	1:B:767:ARG:HB3	2.45	0.42
1:A:95:ILE:C	1:A:97:GLY:H	2.22	0.42
1:A:43:LEU:N	1:A:567:TYR:CD1	2.88	0.42
1:A:595:ILE:HD11	1:A:603:GLU:CB	2.24	0.42
1:B:713:HIS:O	1:B:714:PHE:CB	2.67	0.42
1:B:766:LEU:O	1:B:767:ARG:NH1	2.52	0.42
1:A:182:ARG:HH21	1:A:185:SER:HA	1.83	0.42
1:A:386:GLN:O	1:A:387:LYS:C	2.57	0.42
1:A:430:ARG:HG2	1:A:457:TYR:CE1	2.55	0.42
1:A:473:CYS:HB3	1:A:480:LEU:O	2.20	0.42
1:B:151:GLN:NE2	1:B:168:ASN:H	2.16	0.42
1:B:460:VAL:CG2	1:B:461:SER:N	2.81	0.42
1:A:349:THR:HG22	1:A:593:HIS:HB3	2.00	0.42
1:A:557:ASP:OD1	1:A:561:ARG:NH2	2.52	0.42
1:B:370:TYR:CE2	1:B:384:GLN:CG	3.01	0.42
1:B:430:ARG:HD3	1:B:430:ARG:HA	1.88	0.42
1:B:473:CYS:HB3	1:B:480:LEU:O	2.19	0.42
1:A:389:ARG:CG	1:A:390:LYS:N	2.83	0.42
1:B:152:TRP:O	1:B:164:TYR:HA	2.18	0.42
1:A:346:THR:CG2	1:A:347:SER:N	2.83	0.42
1:B:124:HIS:CE1	1:B:207:GLY:O	2.73	0.42
1:B:277:THR:HG22	1:B:279:THR:H	1.84	0.42
1:B:383:CYS:HB2	1:B:396:THR:C	2.40	0.42
1:B:508:VAL:HG12	1:B:510:MET:HE3	2.02	0.42
1:B:690:MET:CE	1:B:720:ILE:CA	2.98	0.42
1:A:414:ASP:O	1:A:437:LEU:HG	2.19	0.42
1:A:514:LYS:O	1:A:528:GLN:HA	2.20	0.42
1:B:601:THR:HG22	1:B:602:LEU:H	1.83	0.42
1:A:605:GLU:O	1:A:608:ILE:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:511:PRO:HD3	1:B:570:SER:HB2	2.01	0.42
1:A:299:CYS:SG	1:A:314:LEU:HB2	2.60	0.41
1:A:343:HIS:ND1	1:A:394:VAL:HG11	2.36	0.41
1:A:381:HIS:NE2	1:A:399:THR:HG22	2.34	0.41
1:B:120:LYS:CG	1:B:121:GLN:N	2.83	0.41
1:B:658:SER:HB2	1:B:690:MET:SD	2.60	0.41
1:B:92:THR:O	1:B:95:ILE:HG13	2.19	0.41
1:A:418:TYR:O	1:A:432:LEU:HD12	2.20	0.41
1:B:415:TYR:CD2	1:B:436:GLN:HA	2.55	0.41
1:B:458:TYR:HA	1:B:472:GLY:O	2.20	0.41
1:B:469:TYR:OH	1:B:489:GLN:HG3	2.20	0.41
1:B:746:SER:O	1:B:750:GLN:HG3	2.20	0.41
1:B:264:VAL:HG12	1:B:265:LYS:H	1.86	0.41
1:B:329:ASP:HB2	1:B:336:ASN:HD21	1.85	0.41
1:B:533:PRO:C	1:B:535:PHE:H	2.20	0.41
1:A:220:PHE:HB3	1:A:268:ILE:CG2	2.50	0.41
1:A:604:VAL:HG13	1:A:640:VAL:HG23	2.03	0.41
1:A:61:VAL:HG11	1:A:109:ARG:CD	2.51	0.41
1:A:61:VAL:HG11	1:A:109:ARG:HD3	2.02	0.41
1:A:719:GLN:HE22	1:A:722:LYS:HE2	1.85	0.41
1:B:174:ILE:H	1:B:174:ILE:CD1	2.29	0.41
1:B:54:LYS:HB2	1:B:498:ASN:HD21	1.85	0.41
1:A:464:LYS:O	1:A:465:GLU:HG3	2.21	0.41
1:A:690:MET:CE	1:A:720:ILE:N	2.83	0.41
1:B:536:ASP:OD2	1:B:539:LYS:HG3	2.20	0.41
1:B:601:THR:CG2	1:B:602:LEU:H	2.34	0.41
1:B:47:LEU:HD22	1:B:750:GLN:HA	2.03	0.41
1:A:392:GLU:O	1:A:393:GLN:CG	2.69	0.41
1:A:470:GLN:HA	1:A:483:LEU:HA	2.01	0.41
1:B:399:THR:CG2	1:B:403:TRP:CH2	3.03	0.41
1:B:637:THR:HG21	1:B:652:ILE:O	2.20	0.41
1:B:713:HIS:O	1:B:715:GLN:N	2.47	0.41
1:A:144:GLU:O	1:A:173:LYS:NZ	2.52	0.41
1:A:767:ARG:HD2	1:A:767:ARG:OXT	2.21	0.41
1:B:503:LYS:O	1:B:506:GLN:HB2	2.21	0.41
1:B:509:GLN:O	1:B:533:PRO:HG3	2.20	0.41
1:B:536:ASP:HB3	1:B:539:LYS:CE	2.51	0.41
1:B:256:LYS:HZ3	1:B:713:HIS:HD2	1.67	0.41
1:A:690:MET:CE	1:A:719:GLN:C	2.89	0.41
1:A:75:LEU:HB2	1:A:77:PHE:CE1	2.52	0.41
1:B:264:VAL:HG12	1:B:265:LYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:LYS:HB2	1:A:404:GLU:CD	2.40	0.41
1:B:173:LYS:HB3	1:B:173:LYS:HE3	1.80	0.41
1:B:379:TYR:CE2	1:B:402:ALA:HA	2.56	0.41
1:B:447:SER:HA	1:B:450:LEU:CD1	2.50	0.41
1:B:529:MET:HE3	1:B:575:ILE:HG21	2.03	0.41
1:A:533:PRO:CD	1:A:570:SER:HA	2.51	0.41
1:B:273:SER:O	1:B:275:SER:N	2.54	0.41
1:B:390:LYS:HA	1:B:391:PRO:HD2	1.79	0.41
1:B:656:PRO:O	1:B:712:VAL:HG11	2.21	0.41
1:A:240:SER:O	1:B:722:LYS:NZ	2.53	0.40
1:A:306:GLU:HG2	1:A:306:GLU:O	2.21	0.40
1:A:383:CYS:HB2	1:A:396:THR:O	2.20	0.40
1:B:297:TYR:CE1	1:B:316:ARG:HA	2.56	0.40
1:B:349:THR:HG22	1:B:593:HIS:HB3	2.03	0.40
1:A:175:GLU:CG	1:A:178:LEU:HG	2.52	0.40
1:A:517:PHE:CD1	1:A:524:ARG:HD3	2.56	0.40
1:A:652:ILE:HG21	1:A:756:MET:HE2	2.02	0.40
1:A:655:ALA:N	1:A:656:PRO:CD	2.85	0.40
1:B:122:TRP:CE3	1:B:122:TRP:N	2.89	0.40
1:B:639:MET:HE1	1:B:692:ARG:HD2	2.04	0.40
1:A:133:TYR:CE2	1:A:135:LEU:HD23	2.56	0.40
1:A:235:GLU:HG2	1:A:251:TRP:HA	2.03	0.40
1:A:53:VAL:HG22	1:A:501:LEU:HD22	2.03	0.40
1:A:56:TYR:CE2	1:A:495:LEU:HD22	2.56	0.40
1:B:421:ASN:ND2	1:B:427:PRO:HA	2.35	0.40
1:B:497:ASP:O	1:B:499:SER:N	2.52	0.40
1:B:721:SER:O	1:B:725:VAL:HG23	2.21	0.40
1:B:80:GLU:HB3	1:B:81:HIS:H	1.76	0.40
1:A:161:LYS:NZ	1:A:271:THR:CG2	2.85	0.40
1:A:355:PHE:O	1:A:670:ARG:NH1	2.55	0.40
1:A:53:VAL:CG1	1:A:479:PRO:HG3	2.51	0.40
1:B:102:ASP:OD1	1:B:103:TYR:N	2.46	0.40
1:B:138:ARG:C	1:B:139:GLN:HG3	2.42	0.40
1:B:193:PHE:O	1:B:225:GLN:HA	2.21	0.40
1:B:349:THR:HG22	1:B:593:HIS:CB	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	728/730 (100%)	638 (88%)	67 (9%)	23 (3%)	4	16
1	B	728/730 (100%)	634 (87%)	69 (10%)	25 (3%)	3	15
All	All	1456/1460 (100%)	1272 (87%)	136 (9%)	48 (3%)	4	15

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	80	GLU
1	A	143	GLU
1	A	450	LEU
1	A	475	GLY
1	A	533	PRO
1	A	534	HIS
1	A	585	GLY
1	B	80	GLU
1	B	143	GLU
1	B	274	LEU
1	B	450	LEU
1	B	475	GLY
1	B	533	PRO
1	B	534	HIS
1	B	585	GLY
1	A	82	GLY
1	A	91	SER
1	A	92	THR
1	A	318	GLN
1	A	393	GLN
1	A	424	LYS
1	A	498	ASN
1	A	713	HIS
1	B	91	SER
1	B	92	THR

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Mol	Chain	Res	Type
1	B	318	GLN
1	B	393	GLN
1	B	713	HIS
1	A	83	ASN
1	A	147	PRO
1	A	521	ASN
1	B	391	PRO
1	B	442	ASN
1	B	766	LEU
1	A	619	PHE
1	B	147	PRO
1	B	461	SER
1	B	464	LYS
1	B	537	LYS
1	A	343	HIS
1	A	356	ARG
1	A	391	PRO
1	B	83	ASN
1	B	343	HIS
1	B	356	ARG
1	B	619	PHE
1	A	274	LEU
1	B	82	GLY

5.3.2　Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	643/651 (99%)	595 (92%)	48 (8%)	13	37
1	B	643/651 (99%)	601 (94%)	42 (6%)	17	45
All	All	1286/1302 (99%)	1196 (93%)	90 (7%)	15	41

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	84	SER
1	A	94	GLU
1	A	118	TYR
1	A	122	TRP
1	A	139	GLN
1	A	146	ILE
1	A	148	ASN
1	A	175	GLU
1	A	264	VAL
1	A	271	THR
1	A	277	THR
1	A	283	MET
1	A	299	CYS
1	A	300	ASP
1	A	319	ASN
1	A	340	THR
1	A	342	GLU
1	A	346	THR
1	A	356	ARG
1	A	394	VAL
1	A	395	CYS
1	A	414	ASP
1	A	453	GLU
1	A	470	GLN
1	A	483	LEU
1	A	485	ARG
1	A	486	SER
1	A	489	GLN
1	A	518	ILE
1	A	519	VAL
1	A	533	PRO
1	A	547	VAL
1	A	548	TYR
1	A	586	TYR
1	A	595	ILE
1	A	598	ARG
1	A	609	GLU
1	A	624	ARG
1	A	680	ASN
1	A	686	ASN
1	A	688	THR
1	A	690	MET

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Mol	Chain	Res	Type
1	A	698	GLN
1	A	707	THR
1	A	715	GLN
1	A	716	GLN
1	A	767	ARG
1	B	52	ARG
1	B	84	SER
1	B	94	GLU
1	B	118	TYR
1	B	139	GLN
1	B	146	ILE
1	B	148	ASN
1	B	175	GLU
1	B	264	VAL
1	B	271	THR
1	B	277	THR
1	B	299	CYS
1	B	319	ASN
1	B	342	GLU
1	B	346	THR
1	B	394	VAL
1	B	395	CYS
1	B	414	ASP
1	B	453	GLU
1	B	470	GLN
1	B	483	LEU
1	B	485	ARG
1	B	489	GLN
1	B	518	ILE
1	B	519	VAL
1	B	533	PRO
1	B	547	VAL
1	B	548	TYR
1	B	586	TYR
1	B	595	ILE
1	B	598	ARG
1	B	609	GLU
1	B	624	ARG
1	B	664	ASP
1	B	680	ASN
1	B	686	ASN
1	B	688	THR

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Mol	Chain	Res	Type
1	B	690	MET
1	B	707	THR
1	B	715	GLN
1	B	716	GLN
1	B	767	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	90	ASN
1	A	148	ASN
1	A	151	GLN
1	A	319	ASN
1	A	381	HIS
1	A	484	HIS
1	A	498	ASN
1	A	593	HIS
1	A	680	ASN
1	A	683	HIS
1	A	713	HIS
1	A	715	GLN
1	A	716	GLN
1	A	719	GLN
1	A	749	HIS
1	B	49	ASN
1	B	90	ASN
1	B	148	ASN
1	B	151	GLN
1	B	284	GLN
1	B	319	ASN
1	B	336	ASN
1	B	381	HIS
1	B	384	GLN
1	B	484	HIS
1	B	498	ASN
1	B	593	HIS
1	B	607	GLN
1	B	680	ASN
1	B	683	HIS
1	B	713	HIS
1	B	715	GLN

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Mol	Chain	Res	Type
1	B	716	GLN
1	B	719	GLN
1	B	749	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	LIR	A	900	-	23,30,30	1.03	1 (4%)	26,44,44	2.10	10 (38%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LIR	A	900	-	-	3/6/20/20	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	LIR	C25-C20	3.04	1.44	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	LIR	C13-N12-C7	-5.39	110.48	122.03
2	A	900	LIR	C17-N12-C7	-4.26	112.91	122.03
2	A	900	LIR	C4-C3-C2	3.07	108.67	104.66
2	A	900	LIR	C25-C26-N27	-2.67	173.48	177.88
2	A	900	LIR	C16-C15-C14	-2.62	108.55	111.87
2	A	900	LIR	C13-C14-N18	-2.56	106.30	111.60
2	A	900	LIR	C20-C25-C26	2.54	122.57	120.14
2	A	900	LIR	C19-C20-C25	2.53	124.49	120.73
2	A	900	LIR	C20-C19-N6	2.44	117.29	113.26
2	A	900	LIR	C14-C13-N12	2.12	112.31	109.64

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	LIR	C20-C19-N6-C2
2	A	900	LIR	C20-C19-N6-C7
2	A	900	LIR	N6-C19-C20-C21

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	LIR	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand LIR A 900

Bond lengths

Bond angles

Torsions

Rings
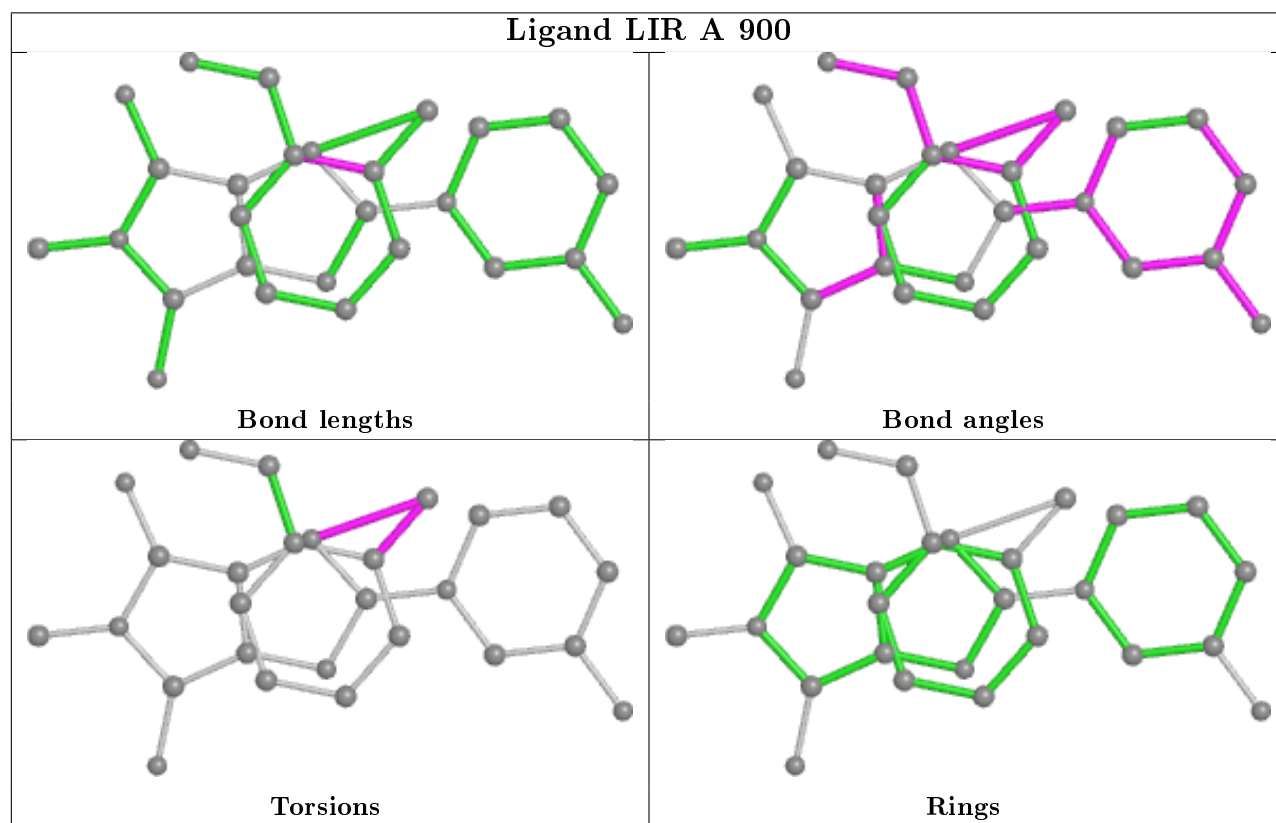
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	730/730 (100%)	-0.22	10 (1%)	75	75	21, 41, 69, 122	0
1	B	730/730 (100%)	-0.09	18 (2%)	57	55	22, 48, 81, 124	0
All	All	1460/1460 (100%)	-0.15	28 (1%)	66	65	21, 44, 75, 124	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	767	ARG	7.2
1	B	392	GLU	3.7
1	B	393	GLN	3.7
1	A	393	GLN	3.7
1	A	251	TRP	3.6
1	A	38	ARG	3.4
1	B	767	ARG	3.1
1	A	392	GLU	3.0
1	B	438	THR	2.9
1	B	138	ARG	2.8
1	B	217	ASN	2.8
1	A	94	GLU	2.8
1	B	72	ASN	2.7
1	B	348	ALA	2.7
1	A	391	PRO	2.5
1	A	98	ASP	2.5
1	B	95	ILE	2.4
1	B	251	TRP	2.4
1	B	439	ASP	2.4
1	B	400	LYS	2.3
1	A	475	GLY	2.2
1	B	444	LYS	2.2
1	B	71	GLU	2.2
1	B	391	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	96	PHE	2.1
1	A	509	GLN	2.1
1	B	507	ASP	2.1
1	B	401	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.
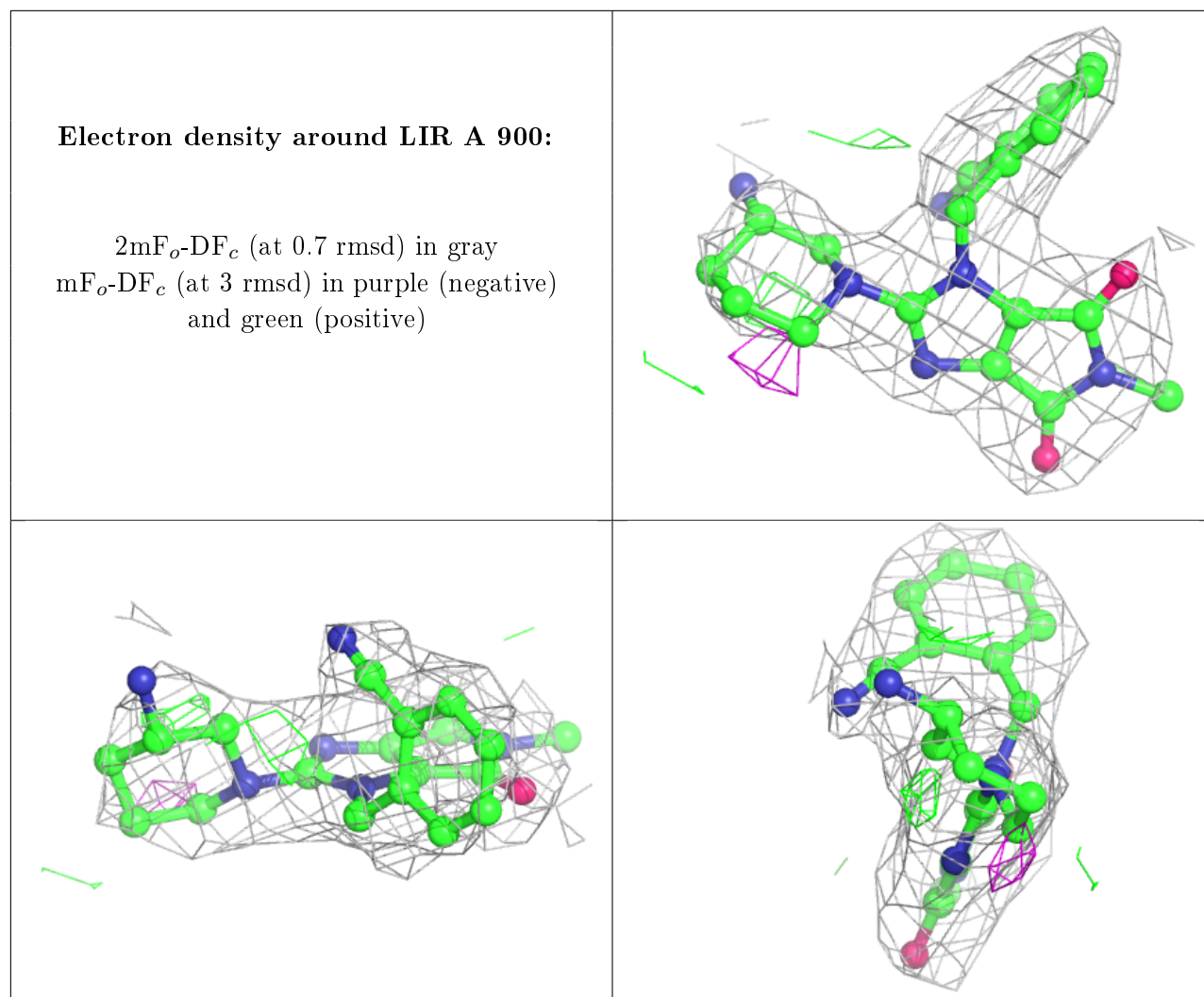
6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LIR	A	900	27/27	0.92	0.25	45,45,45,45	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LIR A 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

6.5　Other polymers ⓘ

There are no such residues in this entry.